LSBR Scientific Advisory Meeting: Computing

NSLS-II, BNL, Upton, NY, March 28 2017
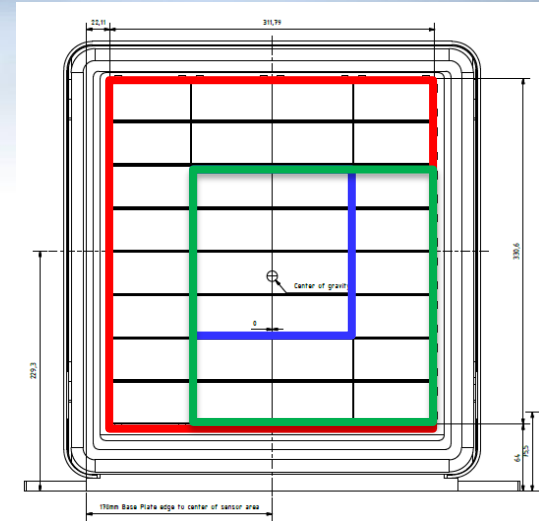
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EIGER 9M @ AMX and 16M @ FMX

Eiger9M
18 modules
10 M pixels
238 Hz

Eiger16M
32 modules
18 M pixels
133 Hz

Eiger 4M ROI
8 modules
4.5 M pixels
750 Hz

233x245	311x328	mm²
238 (750)	133 (750)	Hz
10.2	18.1	M pixel
< 5	< 8	M byte (actual)
200-1700	*200-1700*	MB/s

2-30 TB / day / beamline
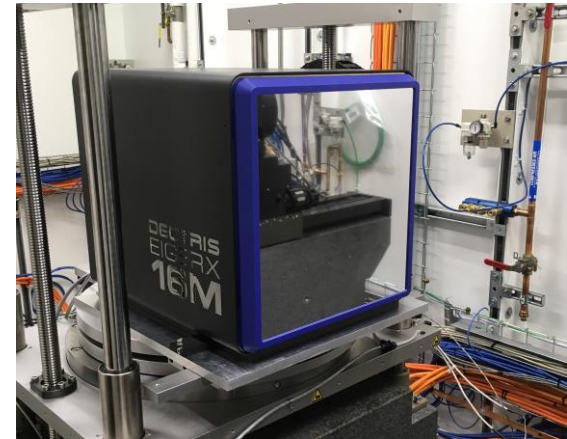
Challenges : data storage, transfer, processing and backup.
Requires advanced software and computing cluster.

AMX / FMX: Current status (275 mA)

AMX : from 5 to 18 keV
Flux > 3×10^{12} ph.s^{-1}
Beam ~ 8 x 7 um^2
Manual sample mounting (up to 10/H)

Typical data collection:
0.1 deg @ 100 Hz
Data collection : from <1s to 15 secs
Default screening:
10 % transmission & 10 ms/frame
Av data set: 1400 frames
500 frames / data.h5
Compression range: 4.2-25
Aver compression:10

FMX : from 5 to 25 keV
Flux > 2×10^{12} ph.s^{-1}
Beam ~ 10 x 6 um^2 (as of last week)
Automated sample mounting (up to 20/H)

Typical data collection:
0.1 deg @ 50 Hz
Data collection : from <1s to 15 secs
Default screening:
<10 % transmission & 50 ms/frame
Av data set: 1800 frames
200 frames / data.h5
Compression range: 4.5-32
Aver compression:11.6

Operate 2 shifts / day, at the moment.

~ 500 GB data per 2 shifts on AMX (at the moment)

Computing / Network Infrastructures

FMX & AMX

9M@AMX

EIGER Detector

16M@FMX

| x controls
Area detector
IOC server
(GPFS / 10 Gb) | 3 x Data Collection Processing Workstations (GPFS / 10 Gb) |

Data collection using LSDC.
Data visualization using Albula or ADSC.
Manual data processing using HKL2000 or other GUIs (ccp4i, phenix, imosflm …),index/Best.
Data transfer onto USB drives.
Direct access to compute nodes over terminal.

40 Gb/s

NSLS-II Computing Facility

Compute Nodes (LSBR)

208 cores
4+4 nodes

GPFS Storage (NSLS-II)

860 TB
IB

GPFS Buffer (LSBR)

20 TB
IB

Rapid Data Analysis and Reduction on dedicated compute nodes and fast buffer
Pipelines and packages in use: dials spot finders, dozor, XDS, dials, xia2, fast_dp, fast_mr, dimple, fast_ep, fast_ep_weak, fast_ep_NSLS-II, KAMO, and more.
Network backup using dedicated node.

10 then 40 Gb/s

> 2000 KNL cores; > 1 PB GPFS

BNL Institutional Cluster

Post processing, Re-processing, Remote processing, Multiple Crystals data reduction and Hierarchical Cluster Analysis.

4

To world (1 Gb/s (internet) to 100 Gb/s (EsNet))

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# Rastering: goal is near real time analysis

1 master/data file per row.
Frames converted (eiger2cbf) and processed with dials.find_spots client / server (ping/pong 2 nodes)
Data located on GPFS

Current performances: processing at ~ 15 FPS on one node
(need to be at ~ 200 E9M FPS, ~ 100 E16M FPS and ~ 500 E4M FPS)

Mixed results when ice rings are present: optimizing dials code and or using dozor (ESRF/EMBL)
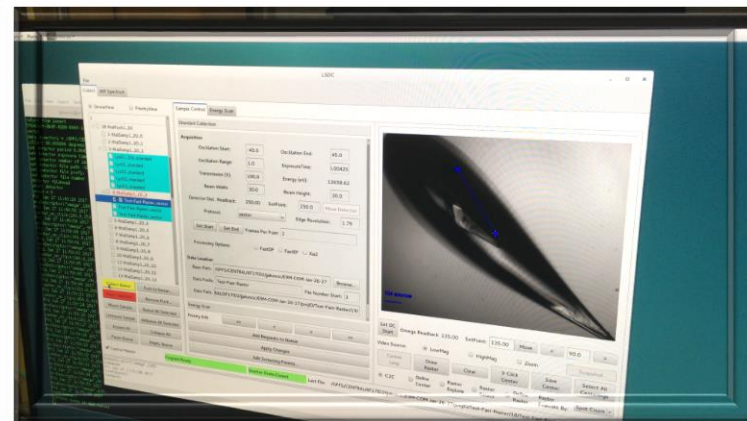
>>>> optimizing codes for faster results (ROI, HDF5 read, KNL, OMP ……)
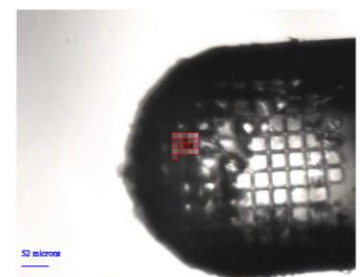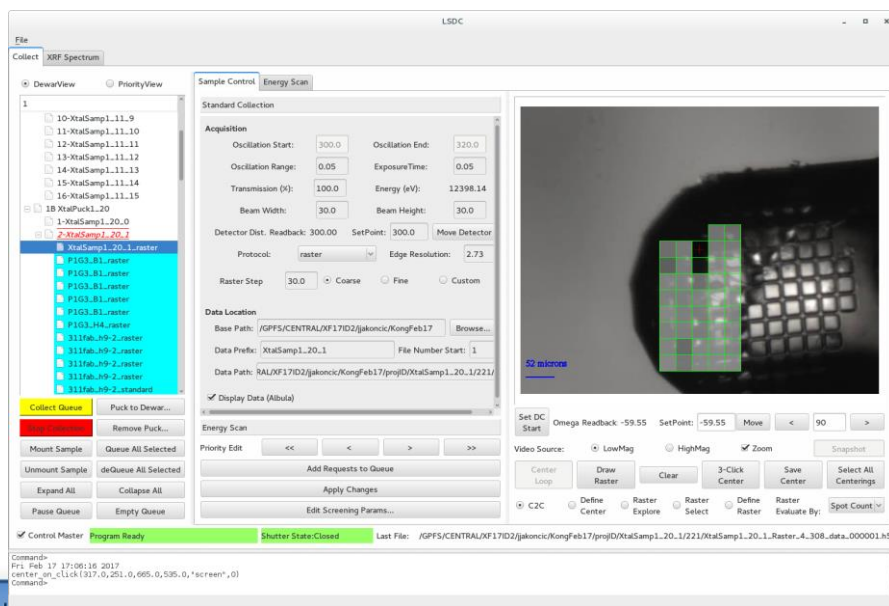
fine

Data Reduction: goal is dataset reduction under 2 min

Fast_dp: on 1 dedicated node (more to be used soon) @ 2-10 FPS.
data set of 900 frames (lysozyme test). (all data on GPFS)

9M	Total time (s)	FPS
FastDP-002	86 (79 RAM)	10 (11)
FastDP-010	83 (50 RAM)	11 (18)
XDS-002	61 (55 RAM)	15 (16)
XDS-010	72 (43 RAM)	12 (21)

XDS: jobs = all, 72 procs, 16 jobs)

Average performances on GPFS
(depending on load: IO dependant)

CPUS 004, 005: 36 cores@2.3 GHz (10 Gb)
CPUs 009, 010: 44 cores@2.2 GHz (40 Gb)
CPUs 002, 003, 007, 008: 12 cores@3.4 GHz (10 Gb)

NetApp EF560 All-Flash Array

20 x 1.6 TB all flash
6 GB/s (50/50)
2 IB controllers 2 ports each

Procured/Delivered/ To be Tested

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Analysis Pipelines

DIMPLE (modified)
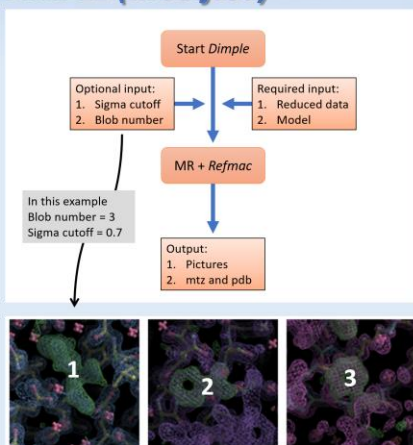
FAST_EP_WEAK

Fast_ep_weak is a modified version of Fast_ep, which is originally developed at Diamond Light Source. Fast_ep_weak is designed to find a structure solution from weak anomalous signals by finer grid searches with spacegroup, nsite and resolution cut off.
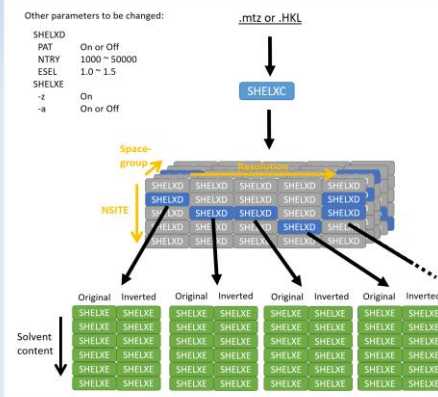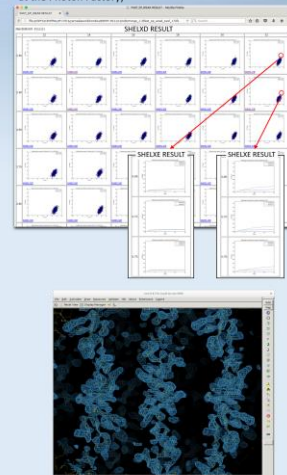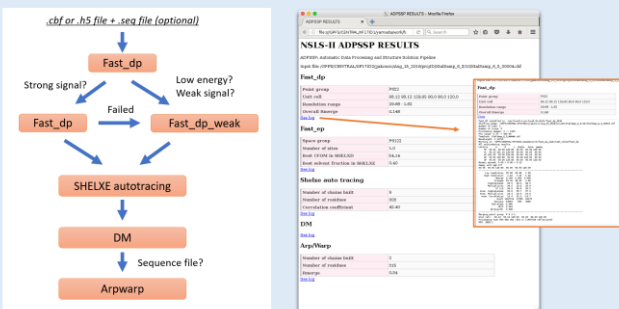

A. Soares, <u>Y. Yamada</u> (PF)
G.Winter (DLS)., H.Bernstein (RIT)

FAST_EP_NSLS2 (NSLS-II ADPSSP)

Fast_ep_nsls2 is a single crystal SAD phasing pipeline from a diffraction data set to a model with fast_dp, fast_ep, fast_ep_weak and other crystallographic software.

Simple report of a processing result

Thermolysin Zn-SAD at AMX at 11 keV

fast_dp (data reduction)	< 150 s	fast_ep	< 200 s
Space group	P622	DF/F	0.049
Unit-cell parameters	a=b=93.13 c= 129.92	dI/sig(dI)	0.898
Mosaicity spread (°)	0.05 < 0.08 < 0.12	Best space group	P6₁22
Resolution (Å)	29.68-1.51 (1.55-1.51)	shelxe_autotrace	6 m
R_merge	0.121 (0.627)	CC (%)	42.42
I/sigma	21.20 (3.30)	Chains	8
Completeness (%)	99.7 (96.6)	Residues	306
Multiplicity	25.1 (12.6)	arpWarp (2 building cycles)	< 130 s
CC(½)	99.9 (88.1)	Residues / water	314 (out of 316) / 0
Anom. Completeness	99.7 (96.0)	R_factor / R_free	0.37 / 0.40
Resolution (Å)	29.68-1.51 (1.55-1.51)	arpWarp (5 building cycles)	< 600 s
R_merge	0.121 (0.627)	Residues / water	315 / 330
I/sigma	21.20 (3.30)	R_factor / R_free	0.22 / 0.25
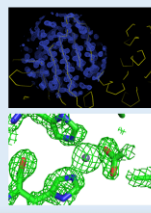
All processing performed on a single node ; total time < 15 mins

KAMO

Multiple small wedge data collection at AMX
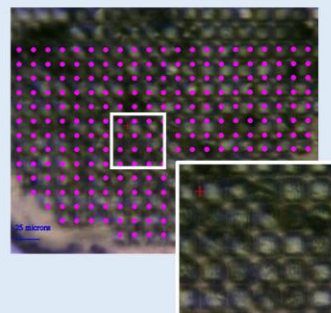
Energy	8
Flux	5.3 x 10¹¹ ph/sec (85 % attenuation)
Total oscillation	5 deg./spot
Osc. width	0.2 deg./frame
Exp. time	0.04 sec./frame (P6M)

(multi.collect on LSDC)
Raster vs raster + threshold

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Collaborations

H. Bernstein (RIT), Y. Yamada (PF), S. Popov (ESRF), G. Bourenkov (EMBL), G. Winter (DLS), N. Sauter (ALS).

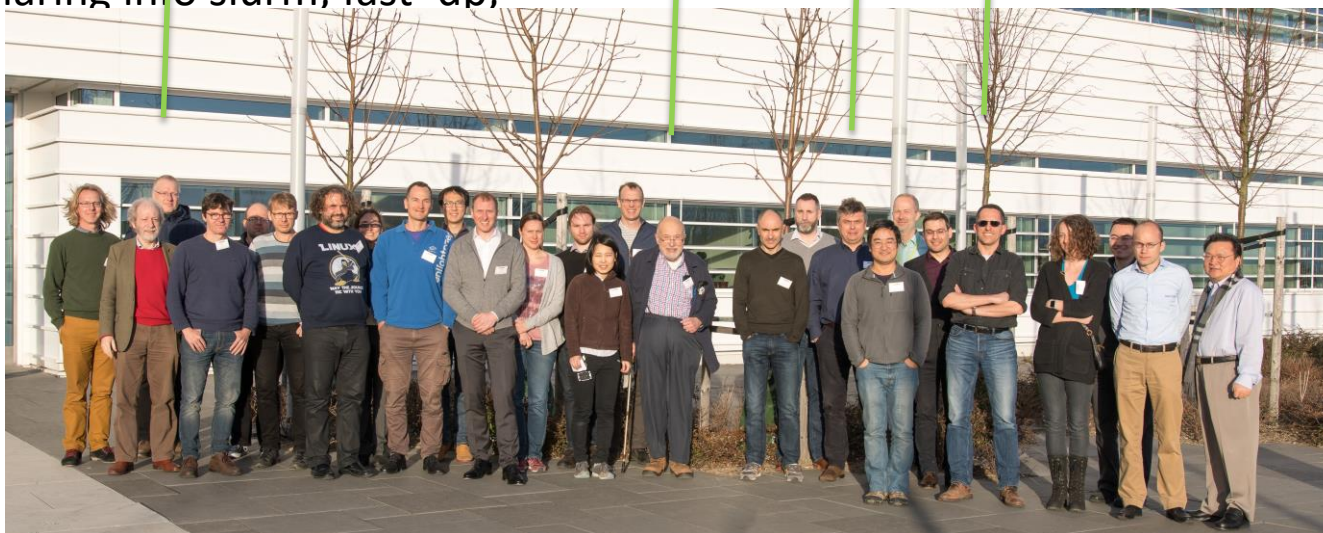Spot finder (dozor and dials): read HDF5 using MP

Indexing (labelit.index) on eiger data producing best files:

Best Strategy on eiger data AND based on data previously processed

> multiple crystals strategy

Data reduction (XDS): parallel colspot, read HDF5 (ram mapping), KNL implementation

HDRMX : sharing info slurm, fast dp,

HDRMX meeting in MAX-IV, Lund (not in picture: Y. Yamada, S. Popov and N. Sauter)

To keep up with the data:

40 Gb/s (infiniband) on all nodes (fast IO) ;
2nd buffer disk (as needed)
Additional compute nodes: > 4 nodes (160 physical cores)
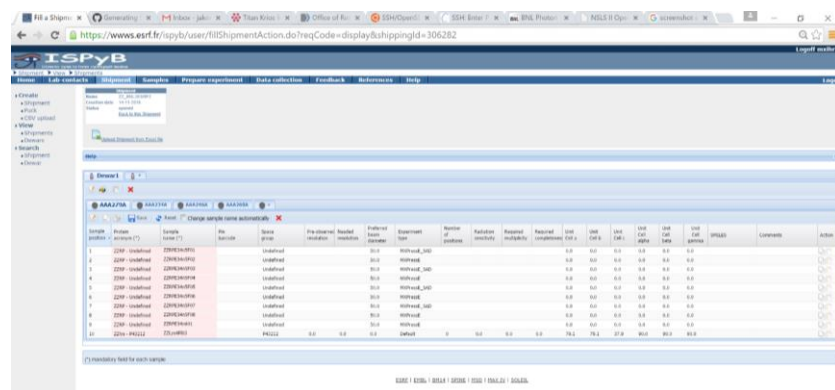
Full slurm deployment (cluster workload management with GPL license)
Database (such as IspyB) is an absolute requirement (Bioinformatics (2011) 27 (22): 3186-3192.);
Users can't keep up with data processing and data quality assessment

Implementation of additional pipelines, specifically for multiple crystals
Using KNLs: spot finder, dozor, xds, dials ? We are testing on Intel cluster: ACA workshop with Intel

Conclusions & Acknowledgements

Data retention: at the moment not an issue (GPFS capacity)

Remote access will be implemented in Summer (NoMachine)

With beams 10 microns or less, we see more head scratching.

Data collection from multiple micro-crystals more and more used.

MR and SAD pipelines are executed manually at the moment (user input required)

Not all users are prepared to handle the amount of data and reprocessing data :
database a must and general cluster with remote access would help.

Learning as we go and implement new features (automation, remote, Multiple crystals data collections, in-situ …

LIX Status: GPFS in use, work in progress with DAMA group.

J. Skinner, B. Martins, R. Petkus, M. Fuchs, A. Soares, E. Lazo.
N. Sauter, G. Winter, S. Popov, G. Bourenkov.
W. Shi, H. Bernstein, Y. Yamada[#].

Save the date:

Open House (Proprietary): April 11

ACA Workshop: May26

NSLS-II: Expert User Training (BAG): 1st ½ June